Schrödinger and Hamilton-Jacobi equations

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Abstract

Time-dependent Schrödinger equation represents the basis of any quantum-theoretical approach. The question concerning its proper content in comparison to the classical physics has not been, however, fully answered until now. It will be shown that there is one-to-one physical correspondence between basic solutions (represented always by one Hamiltonian eigenfunction only) and classical ones, as the non-zero quantum potential has not any physical sense, representing only the "numerical" difference between Hamilton principal function and the phase of corresponding wave function in the case of non-inertial motion. Possible interpretation of superposition solutions will be then discussed in the light of this fact. And also different interpretation alternatives of the quantum-mechanical model will be newly analyzed and new attitude to them will be reasoned.

1. Introduction

Copenhagen quantum mechanics used commonly for the description of microscopic physical processes is based on Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t), \quad H = -\frac{\hbar^2}{2m}\triangle + V(x) \tag{1}$$

and on several additional assumptions. Its predictions differ rather significantly from those of classical physics. And it is possible to ask how much responsibility for different behavior lies already in the Schrödinger equation and how much in the other assumptions.

The question was discussed already earlier and it was assumed that the difference from the classical picture in the Schrödinger equation is given by the existence of the additional quantum potential in one derived equation being analogous to Hamilton-Jacobi equation (see, e.g., Ref. [1]). Some authors tried then to explain the existence of this potential as the consequence of a kind of Brownian motion exhibited by classical microscopic particles [2, 3, 4]. Hoyer showed then that Schrödinger equation may be derived when the classical behavior is combined with the Boltzmann probability [5], and similar approach was proposed earlier also by Ioannidou [6].

We should like to continue in the discussion of the problem in a somewhat different way. Let us assume that a system consisting of N particles is to be described by both the considered equations. To perform more systematic analysis it is then useful to divide the solutions of Schrödinger equation into two different classes:
- basic solutions, when the wave function $\psi(x,t)$ exhibits exponential time dependence and the space part of its is given by one Hamiltonian eigenfunction;
- superposition solutions being formed by different linear superpositions of basic solutions.

The Hamiltonian H represents the total (kinetic + potential) energy of all particles. And it is possible to define their positions and momenta (velocities) in the usual way, i.e.

as expectation values of corresponding operators at any t. The solutions of Schrödinger equation may be then correlated to the solutions of Hamilton equations (see Sec. 2). It will be shown in Sec. 3 that in the case of inertial motion the phase of wave function is quite identical with Hamilton principal function. Non-inertial case will be discussed in Sec. 4; one-dimensional case being analyzed to greater detail. Possible interpretation of superposition solutions that have not any direct counterpart in the classical physics will be discussed in Sec. 5. Different interpretations of quantum-mechanical model in correlation to superposition solutions will be then dealt with in Sec. 6.

2. Relation between Schrödinger and Hamilton-Jacobi equations

The complex wave function fulfilling Eq. (1) may be written in the form

$$\psi(x,t) = \lambda(x,t)\, e^{\frac{i}{\hbar}\Phi(x,t)} \tag{2}$$

and the Schrödinger equation may be substituted by two equations

$$\frac{(\nabla \Phi)^2}{2m} + V + V_q = -\partial_t \Phi, \tag{3}$$

$$\triangle\Phi + 2(\nabla\Phi)(\nabla \lg \lambda) = -2m\, \partial_t \lg \lambda \tag{4}$$

for two real functions: modulus $\lambda(x,t)$ and phase $\Phi(x,t)$. It holds in general case

$$V_q(x,t) = -\frac{\hbar^2}{2m}\frac{\triangle\lambda}{\lambda} \tag{5}$$

and Eq. (3) may be correlated to Hamilton-Jacobi equation

$$\frac{1}{2m}(\nabla S(x,t))^2 + V(x) = -\partial_t S(x,t) \tag{6}$$

where $S(E,t)$ is substituted by $\Phi(x,t)$ and the potential $V(x)$ by

$$V_t(x,t) = V(x) + V_q(x,t); \tag{7}$$

the additional term $V_q(x,t)$ being denoted usually as quantum potential.

3. Equivalence for inertial motion

The Hamilton-Jacobi equation contains Hamilton principle function $S(x,t)$ that determines the momentums of particles in given time:

$$p(x,t) = \nabla S(x,t).$$

And one should ask whether or when the solutions of Schrödinger equation may describe the same physical systems as those of Hamilton-Jacobi equation or what is the difference.

We will limit ourselves to time-independent potential $V(x)$. For the basic solutions of Schrödinger equation it is then possible to write

$$\psi^{(E)}(x,t) = \psi_E(x)e^{-\frac{i}{\hbar}Et}, \tag{8}$$

$$H\psi_E(x) = E\psi_E(x); \tag{9}$$

E is the corresponding energy value, phase $\Phi^{(E)}(x,t) = -Et + \Phi_E(x)$ and modulus $\lambda^{(E)}(x) = \lambda_E(x)$ (see Eq. (2)) is independent of t.

Let us start with the simple case of inertial motion of one particle, i.e., by putting $V(x) \equiv 0$. It holds then

$$\Phi^{(E)}(x,t) = -Et + x\sqrt{2mE}, \quad \lambda_E(x) = 1;$$

and consequently, $V_t = V_q = 0$. It holds also

$$S(x,t) = \Phi(x,t),$$

which means that the constant particle momentum equals

$$p = \frac{\partial S(x,t)}{\partial x} = \frac{\partial \Phi_E(x)}{\partial x}.$$

4. Basic solutions with separated x- and t-dependencies

In a more general case, when $V(x) \neq 0$, there is a certain difference between $S(x,t)$ and $\Phi(x,t)$ as the additional potential term $V_q(x)$ may be non-zero. Let us limit to the basic solutions represented by Eqs. (8) and (9) and let us write

$$\psi_E(x) = \lambda_E(x)e^{\frac{i}{\hbar}\Phi_E(x)}.$$

It is then possible to put

$$\mathbf{P}_E(x) = \nabla\Phi_E(x);$$

for basic solutions it holds also

$$\mathbf{P}_E(x) = \nabla\Phi^{(E)}(x,t).$$

Eq. (4) may be then rewritten as

$$\triangle\Phi_E(x) + 2\,\mathbf{P}_E(x).\nabla\lg\lambda_E(x) = 0 \qquad (10)$$

and the function $\lambda_E(x)$ might be determined with the help of $\Phi_E(x)$ or of $\mathbf{P}_E(x)$ components.

The last equation might be easily solved in *one-dimensional* case. It should hold then

$$\lambda_E(x) = P_E^{-1/2}$$

as $\partial_x^2\Phi_E(x) = \partial_x P_E(x)$. It might lead, however, in some cases to unacceptable behavior (e.g., in the case of an oscillating system the quantum potential would be divergent in some points) which may be avoided in one-dimensional case only if $\Phi_E(x) = const$; Eq. (4) loosing any sense. And the function $\lambda(x)$ (or quantum potential) may be established in such a case on the basis of Eq. (3) with the help of the condition

$$\frac{\partial_x^2\lambda_E(x)}{\lambda_E(x)} = \frac{2m}{\hbar^2}(E - V(x)). \qquad (11)$$

E.g., in the case of one-dimensional harmonic oscillator it holds for individual quantum numbers n:

$$\frac{\partial_x^2 \lambda_n(x)}{\lambda_n(x)} = -\frac{2m}{\hbar^2}[(n + \frac{1}{2})\hbar\omega - \frac{m\omega^2}{2}x^2], \tag{12}$$

which may be verified when $\lambda_n(x)$ is derived from the eigenfunctions of corresponding Hamiltonian.

The solution in a more-dimensional case represents, of course, more complicated problem. One may expect, however, similar results to be obtained.

The quantum potential goes always to zero if the motion of all involved objects is inertial, i.e., if any forces do not act between them. It is non-zero in the case of non-inertial motion, depending on corresponding characteristics of individual physical states. It represents the diference between Hamilton principal function $S(x,t)$ (fulfilling Eq. (6)) and the phase $\Phi(x,t)$ of wave function (fulfilling Eq. (3)) that are expressed by identical functions in the case of inertial motion.

The quantity $\nabla\Phi_E(x,t)$ fulfilling the condition

$$(\nabla\Phi_E(x))^2 = 2m\,(E - V_t(x)) \tag{13}$$

does not represent the momentum components of corresponding particle in non-inertial case; $V_t(x)$ being defined by Eq. (7). And the quantum potential has not practically any actual physical sense.

5. Superpositions of basic solutions

It has been shown in Sec. 4 that the basic solutions of Schrödinger equation may be correlated to corresponding solutions of Hamilton-Jacobi equation; both representing the same physical behavior. There is, however, a difference; any superposition of basic solutions is again a solution of Schrödinger equation, which has not its analogue as to Hamilton-Jacobi equation. It follows from the fact that the Hamilton-Jacobi equation is non-linear differential equation, while the Schrödinger equation is linear differential equation.

Let us assume now that the given set of solutions belongs to continuous energy spectrum. It means that any superposition of basic states must correspond to energy E lying in the same energy spectrum, but representing a different state than the corresponding basic solution. It cannot be characterized by any Hamilton principal function and described as a direct solution of Hamilton-Jacobi equation. And one should ask what is the difference between the basic solutions (corresponding to classically moving particles) and their superpositions, and how to interpret these superpositions physically.

Individual superpositions may hardly represent simple physical states with given energy values. The superpositions of different basic states of Schrödinger equation may provide, however, an advantage in describing measurement results concerning microscopic objects. Any measurement of such a type is based in principle on studying mutual collisions between microscopic particles or interactions of these particles with a macroscopic device. In both the cases the exact classical description would require to know the value of impact parameter between mutually colliding microscopic particles or between a microscopic particle and a collision center in the microscopic structure of a macroscopic object

(i.e., the value of the corresponding "hidden" parameter in the quantum-mechanical picture).

However, the impact parameter is always statistically distributed, even if the other physical properties are the same; e.g., the initial kinetic energy (or momenta) of mutually colliding objects. One cannot determine exactly mutual initial positions of colliding particles in the direction perpendicular to particle tracks. Consequently, it is also the total energy (i.e., the sum of kinetic and potential energies) that is statistically distributed. The dependence on the value b of impact parameter in individual events is given in principle by the shape of mutual potential function $V(b)$. Statistical distributions of other physical characteristics may, of course, contribute to the distribution of the total energy value E, too.

To describe such a situation with the help of Hamilton-Jacobi equation must be denoted, of course, as practically impossible. It would be necessary to sum (or to integrate) individual solutions in agreement with a statistical weighting function. The final result may be obtained, of course, directly by solving Schrödinger equation with the initial function $\psi_0(x)$ given by a corresponding statistical superposition of basic states:

$$\psi_0(x) = \int dE\, c(E)\, \psi_E(x), \quad \int dE\, c^*(E)\, c(E) = 1 \qquad (14)$$

where $\psi_E(x)$ fulfills Eq. (9) and the weighting function $c(E)$ characterizing the corresponding superposition may be real. One general solution of Schrödinger equation may represent, therefore, the statistically distributed result of the whole measurement process concerning microscopic objects.

The collision processes in considered experiments (i.e., mutually colliding free particles at a given energy E) may be described by eigenstates belonging to continuous Hamiltonian spectrum. In the case of bound states the eigenvalue spectrum is discrete, but individual basic states correspond to the solutions of Hamilton-Jacobi equation, forming a subset of classically admitted continuous set of solutions.

And it is the Schrödinger equation that corresponds better than Hamilton-Jacobi equation to experimental data in the microscopic region. Consequently, on the microscopic level the Schrödinger equation should be preferred to classical description. However, the Schrödinger equation may be applied in principle also to physical systems with high energy values (including classical systems) without assuming the Planck constant (being of general validity) to change its value. The differences between the admitted energy values will be so small that it will not be possible to register them at all.

6. Superposition solutions and different interpretations of quantum-mechanical mathematical model

As to the quantum mechanics there are two different interpretations of solutions of Schrödinger equation being discussed in literature all the time: orthodox (Copenhagen) or statistical (ensemble); see, e.g., [7]. In the latter case one may assume, that a superposition solution describes measurement process when an amount of identically prepared microscopic systems is measured, each of them being characterized by different values of some randomly distributed hidden parameters (e.g., impact parameter as discussed in Sec. 5). The corresponding result may be, therefore, easily obtained with the help of

Schrödinger equation if the initial state is expressed as corresponding superposition of basic states (see Eq. (14)).

As to the former interpretation two other important assumptions have been added to the basic Schrödinger equation:
- all solutions of its have been assumed to be represented by vectors in the standard Hilbert space that has been spanned on one set of Hamiltonian eigenfunctions;
- the superposition principle (holding in any mathematical metric space) has been interpreted as the physical property of a described physical system.

It follows from these additional assumptions that any vector of the given Hilbert space must represent a physical state, which leads to an important contradiction concerning experimental data for bound states. As already mentioned in Sec. 5 it follows from Schrödinger equation that the corresponding basic states form a set of discrete states only. However, according to additional Copenhagen assumptions all superpositions (exhibiting continuous spectrum in the whole corresponding energy interval) should exist, too, which contradicts experimental facts.

Some discrepancy between the Schrödinger equation and the additional assumptions of Copenhagen model was indicated by Pauli [8] already in 1933. He showed that the time dependence following from Schrödinger equation may be represented fully in the given standard Hilbert space only if the Hamiltonian exhibits the spectrum of all real values from $-\infty$ to $+\infty$. Many attempts of removing this deficiency have been done in the past, but they have not been successful.

It has been shown only recently (see [9, 10]) that the criticism of Pauli may be removed if the standardly used Hilbert space is extended (doubled). It should consist from two mutually orthogonal simple Hilbert spaces (discussed already earlier by Lax and Phillips [11, 12]), which, e.g., in the case of two free particles may be interpreted as subspaces corresponding to incoming or outgoing states.

Then, of course, all classically required parameters should be included in the description of any physical system in an equivalent way as other characteristics; e.g., also the impact parameter in the case of two particles even if actual measurement may concern the set of systems exhibiting statistically distributed values. The latter interpretation of Schrödinger equation is then in full harmony with the model based on the extended Hilbert space and all superpositions of basic states should be interpreted as considered in Sec. 5.

7. Conclusion

Schrödinger's discovery has consisted in that it has been possible to describe simple classical systems alternatively with the help of the wave equation. Schrödinger demonstrated it practically in the case of inertial motion. It has been shown in the preceding that it holds for any basic states, i.e., for all solutions of Schrödinger equation characterized by one eigenfunction of Hamiltonian only.

The general solutions of Schrödinger equation (i.e., superpositions of basic solutions) may be then made use of in describing statistically distributed results of measurement processes concerning microscopic objects. One superposition solution may represent the statistical result of a whole measurement process if the weighting function is correspondingly chosen. That is in full agreement with the results of Hoyer [5] and Ioannidou [6]

who have shown that Schrödinger equation may be derived if the classical behavior is combined with a kind of statistical distribution.

And one must ask if the time has not come when it is necessary to put the question whether the statistical (ensemble) interpretation of quantum mechanics (i.e., the Schrödinger equation alone) should not be preferred generally and earlier additional assumptions involved in the orthodox (Copenhagen) quantum mechanics abandoned.

The difference in the mathematical model in such a case would consist in the extension (doubling) of the standardly used Hilbert space as shown in [9, 10]. And it is also the mathematical superposition principle that may be hardly interpreted in a physical sense. Otherwise, nothing else would change in the earlier approach based on Schrödinger equation, including the existence of discrete bound states and other quantum characteristics.

References

[1] D. Bohm: A suggested interpretation of the quantum theory in terms of "hidden variables"; *Phys. Rev.*, Vol. 85, (1952), pp. 180-93.

[2] E. Nelson: Derivation of the Schrödinger equation from Newtonian Mechanics; *Phys. Rev.*, Vol. 150, (1969), pp. 1079-85.

[3] L.de la Peña-Auerbach: New formulation of stochastic theory and quantum mechanics; *Lett. Math. Phys.*, Vol. 10 (1969), 1620-9.

[4] L. Smolin: Matrix models as non-local hidden variables theories; *"Quo vadis quantum mechanics?"* (eds. A.Elitzur et al.), Springer, 2005, pp. 121-52.

[5] U. Hoyer: *Synthetische Quantentheorie*; Georg Olms Verlag, Hildesheim, 2002.

[6] H. Ioannidou: A new derivation of Schrödinger equation; *Lett. al Nuovo Cim.*, Vol. 34, (1982), pp. 453-8.

[7] D.Home, M.A.B.Whittaker: Ensemble interpretations of quantum mechanics. A modern perspective; *Phys. Rep. C*, Vol. 21(1992), 223-317.

[8] W.Pauli: Die allgemeinen Prinzipien der Wellenmechanik; *Handbuch der Physik XXIV*, Springer, Berlin 1933, p. 140.

[9] P.Kundrát, M.Lokajíček: Three-dimensional harmonic oscillator and time evolution in quantum mechanics; *Phys. Rev. A*, Vol. 67, (2003), art. 012104.

[10] P.Kundrát, M.Lokajíček: Irreversible time flow and Hilbert space structure; *New Research in Quantum Physics* (eds. Vl.Krasnoholovets, F.Columbus), Nova Science Publishers, Inc., 2004, pp. 17-41.

[11] P.D.Lax, R.S.Phillips: *Scattering theory*; Academic Press, New York, 1967.

[12] P.D.Lax, R.S.Phillips, *Scattering theory for automorphic functions* (Princeton 1976)